Supporting Information

Probing the C-O bond-formation step in metalloporphyrin catalyzed C-H oxygenation reactions

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Section S1: Experimental Details

General information

All manganese porphyrins were synthesized according to literature methods.[1] Normalized $^{18}O_2$ (97% enrichment) was purchased from Cambridge Isotopes Laboratories. Bicyclo[4.1.0] heptane (norcarane), bixanthene and *S*-(1-deuterioethyl)-benzene were prepared according to literature methods.[2] Tetrabutylammonium hydroxide (TBAH), Tetrabutylammonium fluoride (TBAF), *cis*-decalin, xanthene, xanthydrol, xanthone and *m*-chloroperoxybenzoic acid (mCPBA) were purchased from Aldrich. *m*CPBA was purified by washing with pH = 7.4 phosphate buffer. Water was distilled and deionized with a Millipore system.

Instrumentation.

UV-Vis spectra were collected on an Agilent 8453 diode array spectrophotometer using 1 cm quartz cuvettes at room temperature. Products were analyzed on an Agilent 7890A gas chromatography with an Agilent 5975 mass spectrum detector (GC/MS).

General procedure of oxidation reactions

Manganese porphyrin (7 mmol), TBAH or TBAF (indicated equiv. to manganese porphyrin), substrates (550 mmol) and 2 mL solvent (CH_3CN or 1:1 CH_2Cl_2/CH_3CN) was charged in a 4mL vial. The mixture was deaerated by freeze-thawn cycle for three times followed by injection of a deaerated solution of *m*CPBA (55 mmol) in 0.5 mL CH_3CN or 1:1 DCM/CH_3CN under nitrogen. The reaction was stirred for 10 min. After the reaction is done, manganese porphyrin and additive were removed by a short silica gel column eluted by CH_2Cl_2. The eluted CH_2Cl_2 solution was analyzed directly by GC/MS. For ^{18}O label experiment, the reaction was run under the atmosphere of $^{18}O_2$ and the ^{18}O composition in xanthone were analyzed by relative abundance of m/z = 196.1 for xanthone-^{16}O and m/z = 198.1 for xanthone-^{18}O.

Section S2: Computational Details

The geometry optimizations and zero-point vibrational energy (ZPVE) were carried out using the B3LYP[3-5] functional with the 6-31G**[6,7] basis set for all atoms except Mn. For Mn the first four shells of core electrons were described by the Los Alamos angular momentum projected effective core potential (ECP) using the double-ζ contraction of valence functions[8] (denoted as LACVP**) leading to 15 explicit electrons for neural Mn. In order to obtain a more accurate electronic energy, we performed single-point energy calculations based on the same functional, but using a larger basis set, where Mn was described with the triple-ζ contraction of valence functions augmented with two *f* functions[9] (the core electrons were described by the same ECP), with the other atoms described with the 6-311^{++}G**[10,11] basis set.

Solvation energies G(solv) were calculated using the Poisson-Boltzmann self-consistent polarizable continuum method[12,13] implemented in Jaguar to represent CH_2Cl_2 (dielectric constant = 8.93 and effective radius = 2.33 Å). The solvation calculations used the B3LYP/LACVP** level of theory and the gas-phase optimized structures. All energies discussed in this work are E(SCF) + G(solv). Shaik and Nam have used E(SCF) + G(solv) in their theoretical studies to investigate the tendency of the radical recombination or dissociation in several non-heme systems, and the results are consistent with their own experiments.[14]

Section S3: **Supplementary tables and figures**

Representative GC traces of norcarane, *cis*-decalin and xanthene oxidations

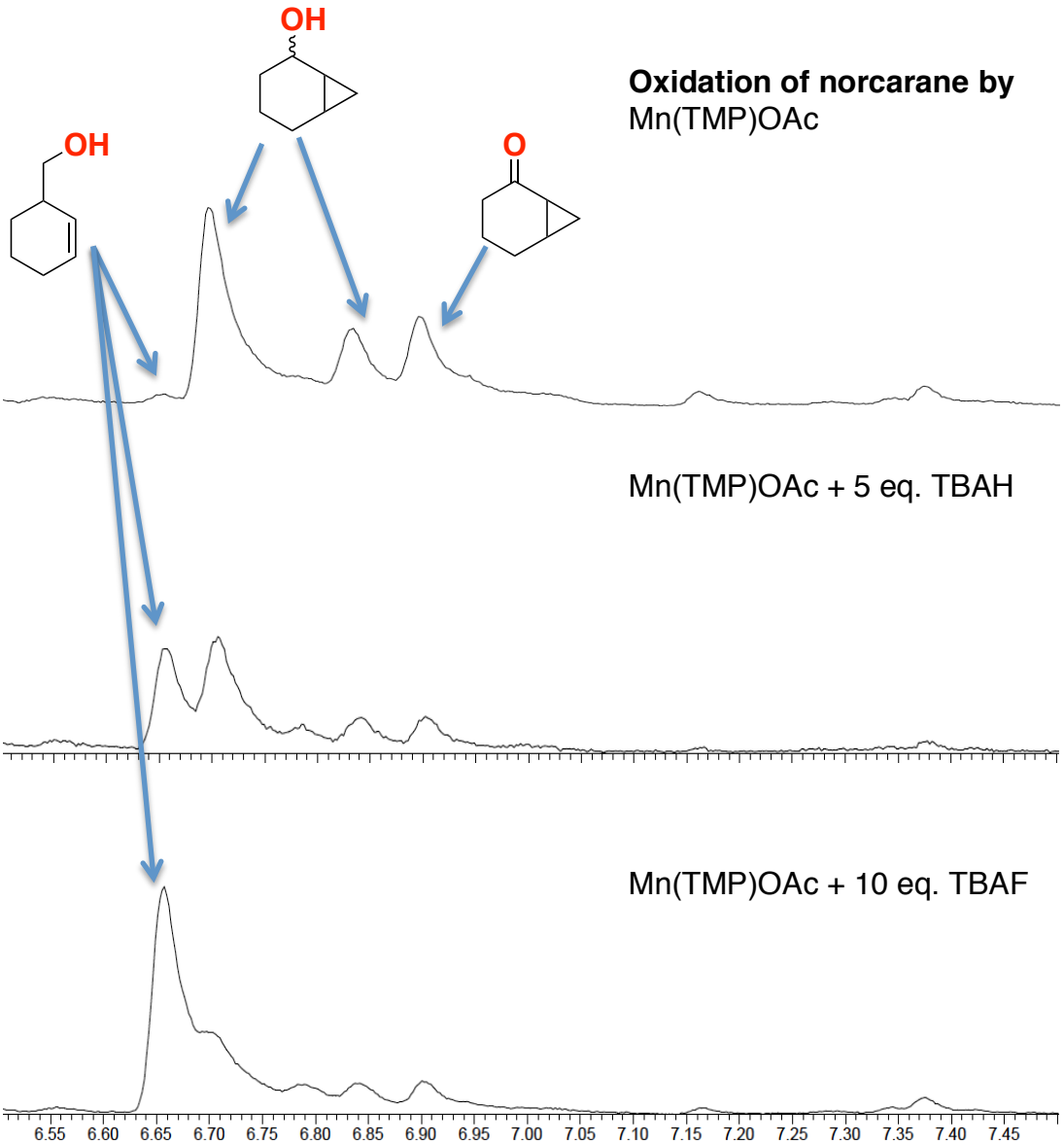


Figure S1. GC traces of norcarane oxidation catalyzed by Mn(TMP)OAc in the presence of TBAH or TBAF

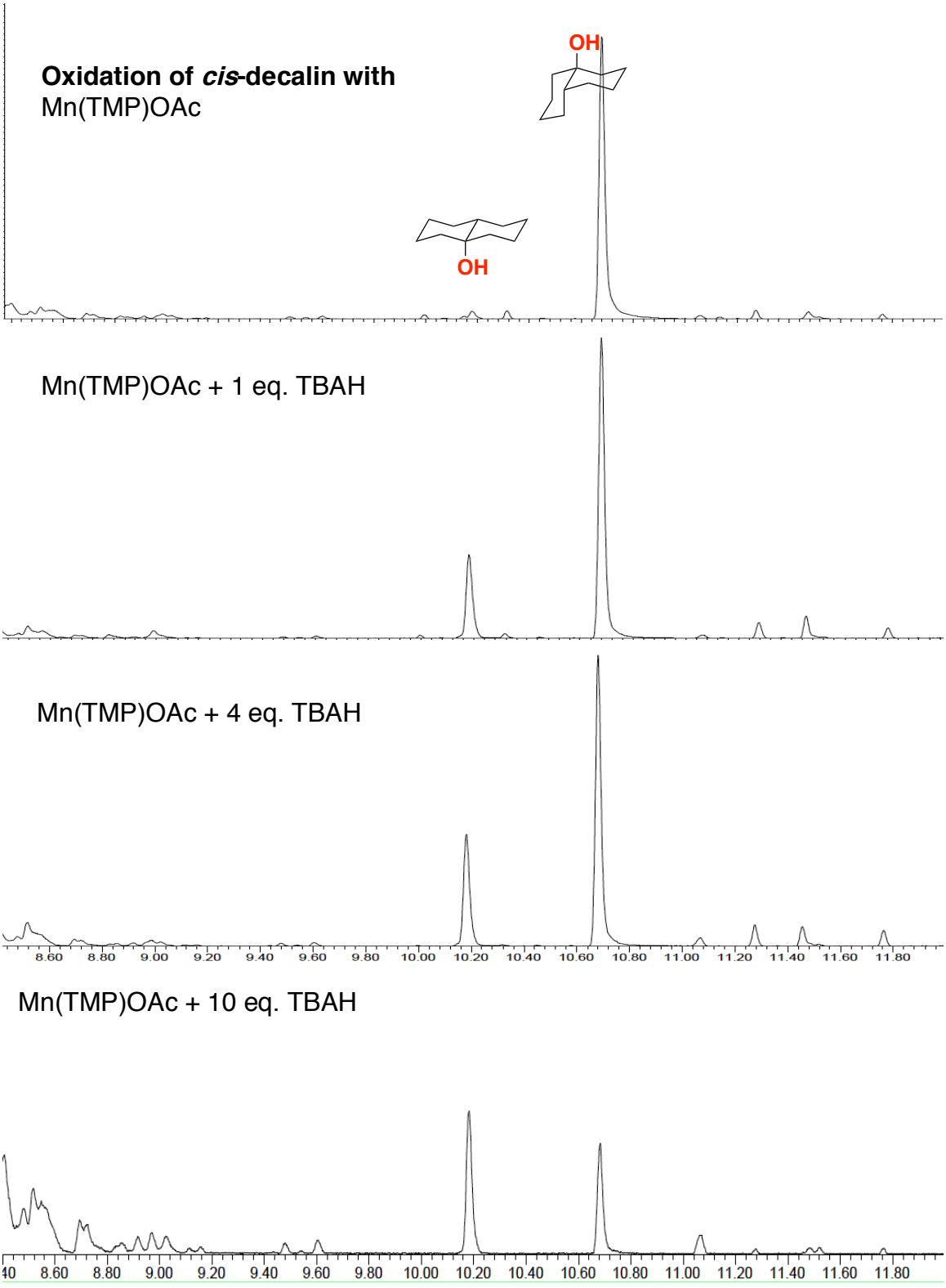


Figure S2. GC traces of *cis*-decalin oxidation of catalyzed by Mn(TMP)OAc in the presence of TBAH

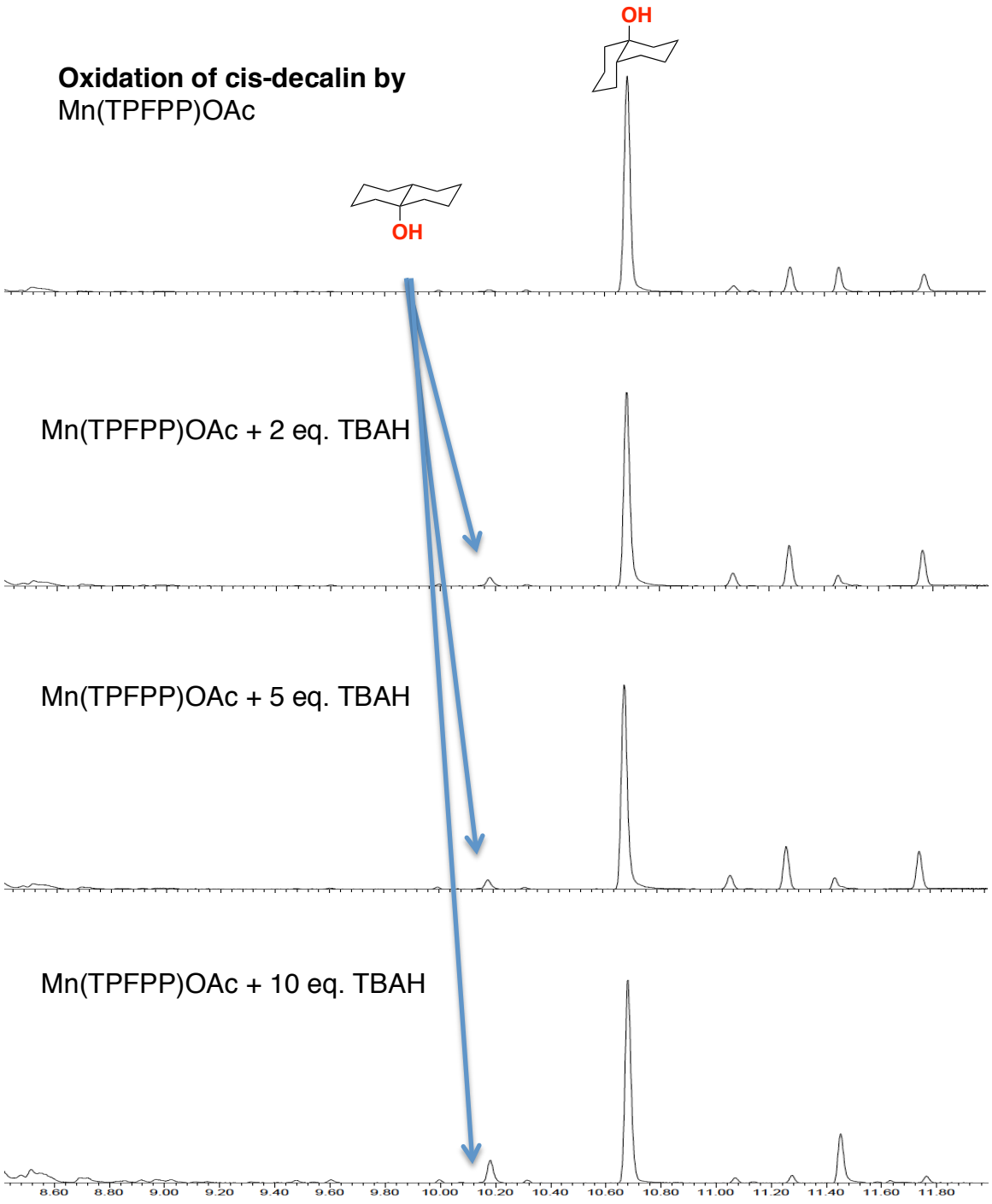


Figure S3. GC traces of *cis*-decalin oxidation catalyzed by Mn(TPFPP)OAc in the presence of TBAH

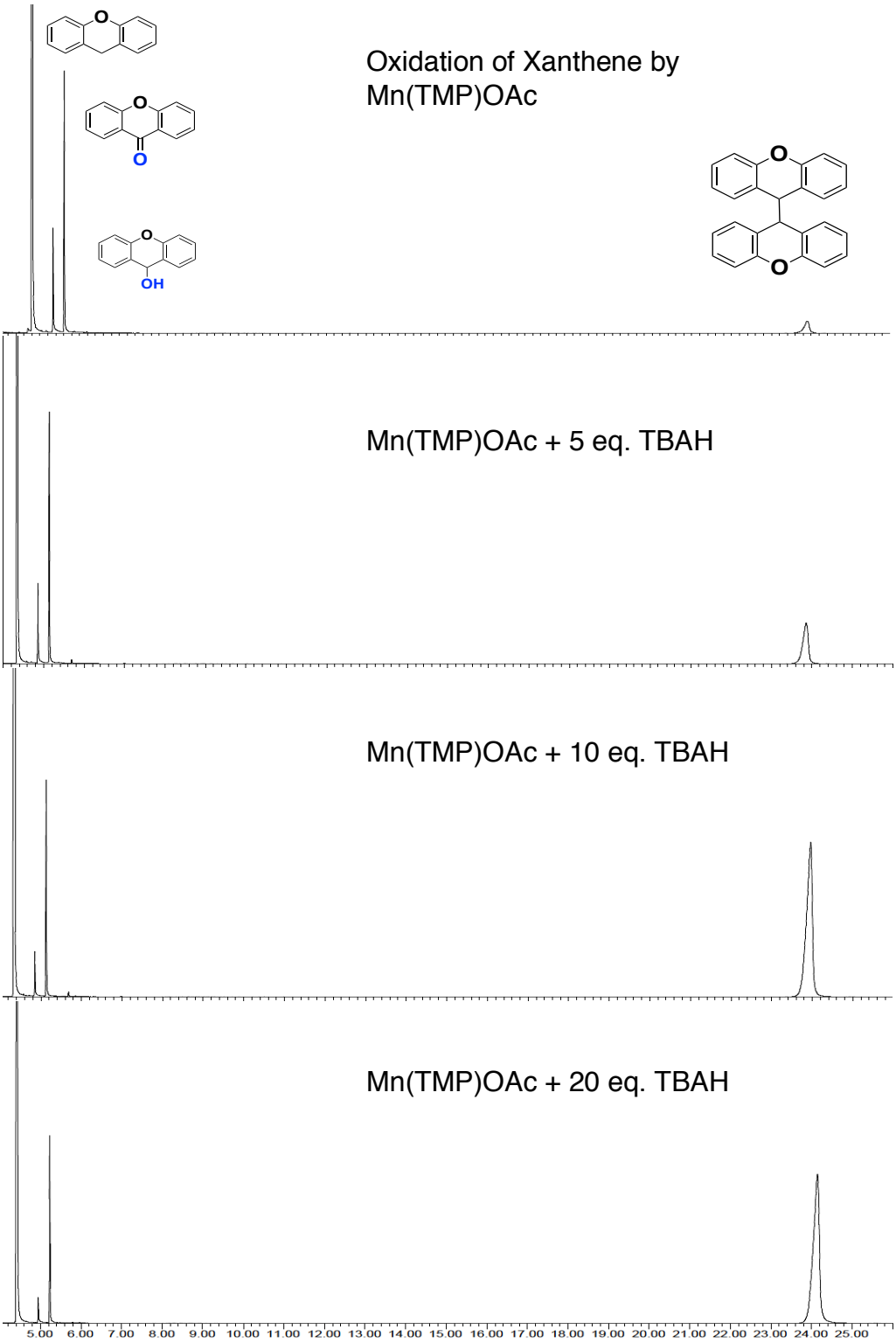


Figure S4. GC traces of xanthene oxidation catalyzed Mn(TMP)OAc in the presence of TBAH

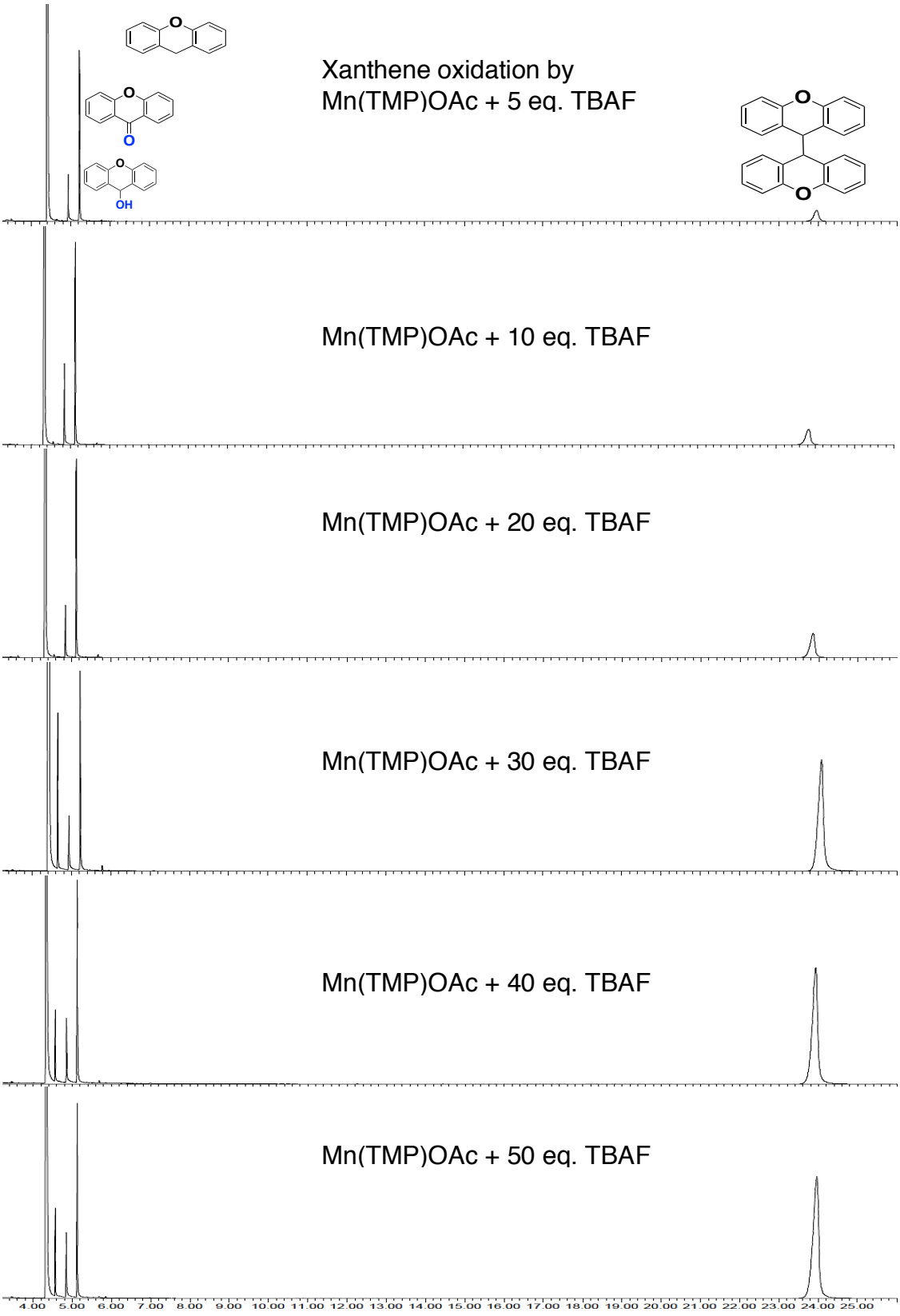


Figure S5. GC traces of xanthene oxidation catalyzed by Mn(TMP)OAc in the presence of TBAF

Table S1. anaerobic oxidation of xanthene[a]

entry	porphyrin	additive	Equiv. of additive	ratio[b]
1	Mn(TPP)OAc	-	-	<0.01
2	Mn(TPP)OAc	TBAF	5	0.23
3	Mn(TPP)OAc	TBAF	10	0.30
4	Mn(TPP)OAc	TBAF	20	0.61
5	Mn(TMP)OAc	-	-	<0.01
6	Mn(TMP)OAc	TBAH	5	1.1
7	Mn(TMP)OAc	TBAH	10	6.1
8	Mn(TMP)OAc	TBAH	20	7.3
9	Mn(TPFPP)OAc	-	-	<0.01
10	Mn(TPFPP)OAc	TBAH	5	0.1
11	Mn(TPFPP)OAc	TBAH	10	0.86
12	Mn(TPFPP)OAc	TBAH	20	7.6

[a]reaction was carried out in CH_2Cl_2/CH_3CN(1:1) under nitrogen. [b.] ratio refers to bixanthene/(xanthydrol+xanthone)

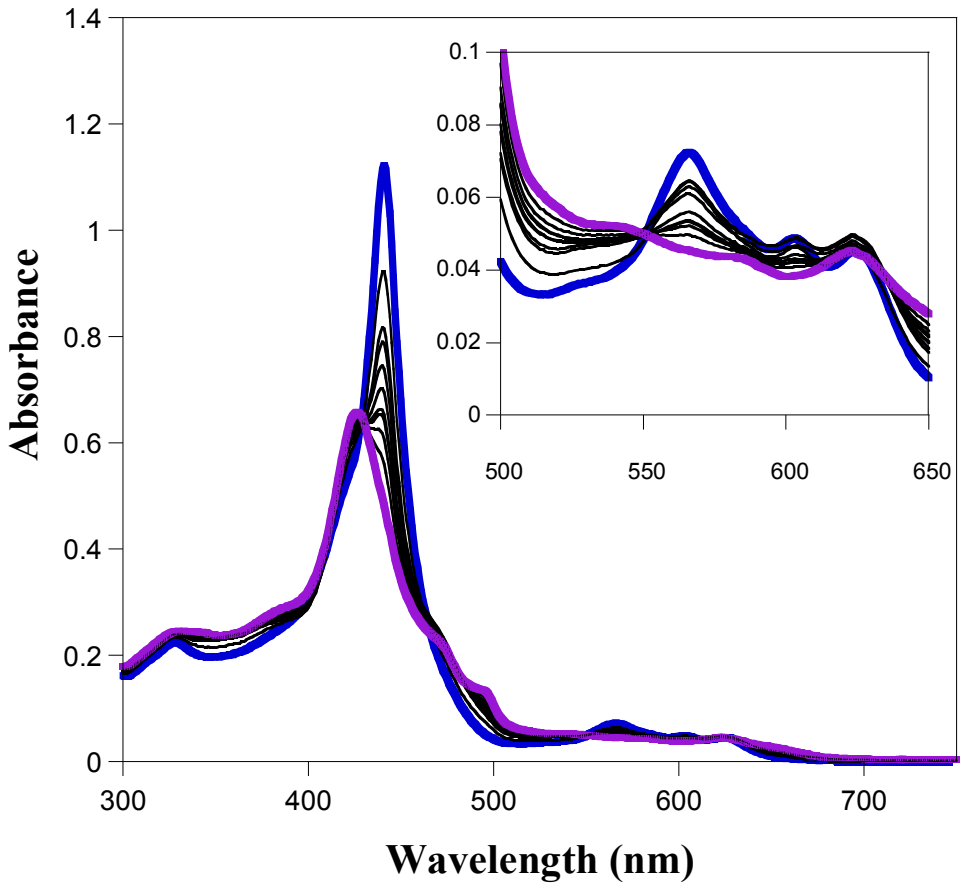


Figure S6. UV-vis spectral changes of $Mn^{V(}TMP)(O)_2$ (blue line) to a $[O=Mn^{IV}(TMP)\text{-}OH]^-$ species (**a**, purple line) upon addition of 100 equiv. xanthene in CH_2Cl_2-CH_3CN (1:1) mixture. Inset shows a magnification of the Q-band region of the manganese porphyrin.

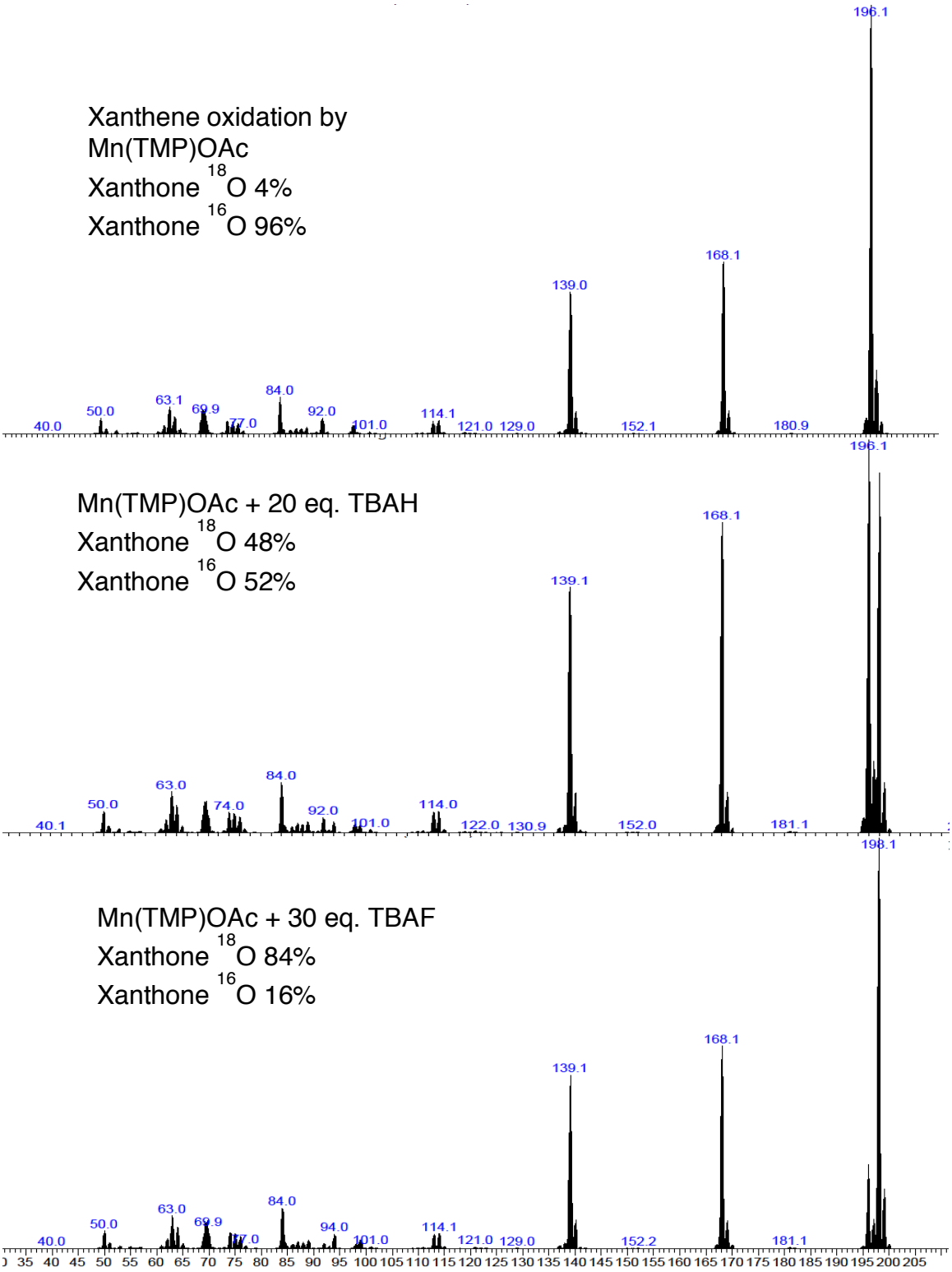


Figure S7. MS spectra of xanthone in $^{18}O_2$ labeling oxidation of xanthene by Mn(TMP)OAc with *m*CPBA in CH_2Cl_2-CH_3CN (1:1). Reactions (a) were carried out in the absence of extra additives, (b) in the presence of 30 equiv. TBAF and (c) in the presence of 20 equiv. TBAH.

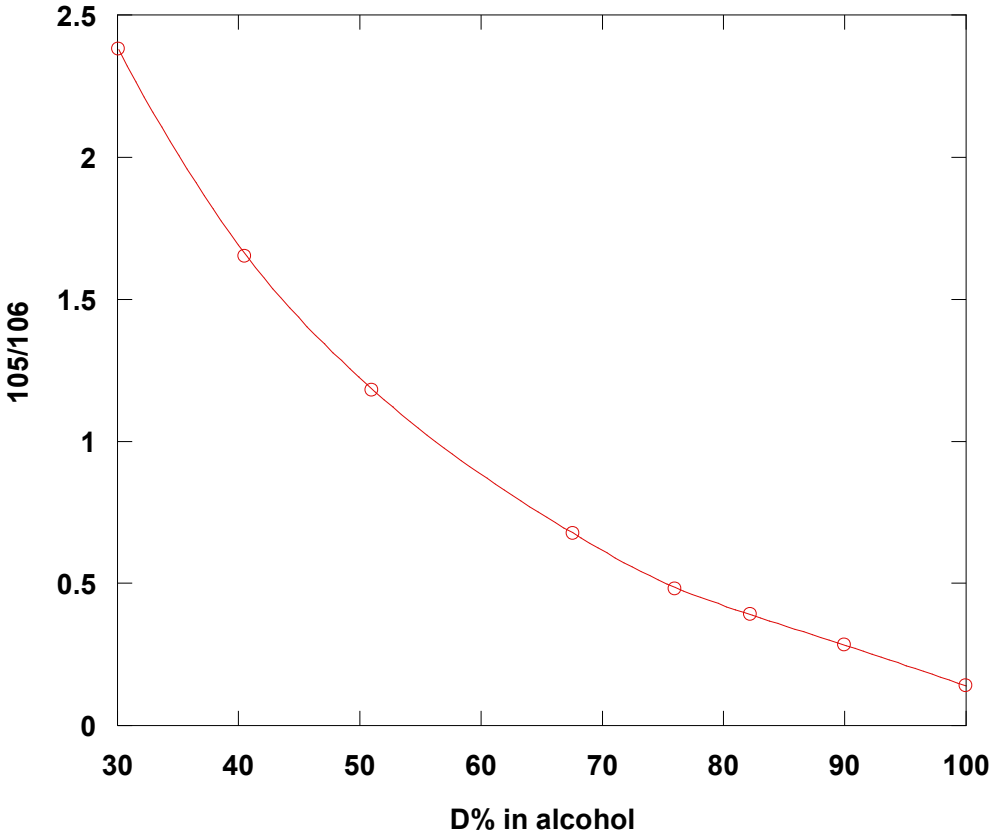
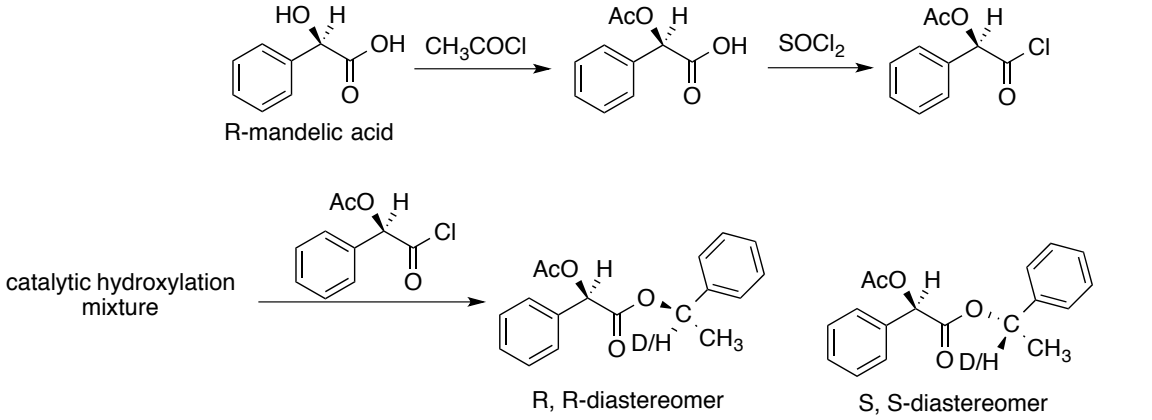
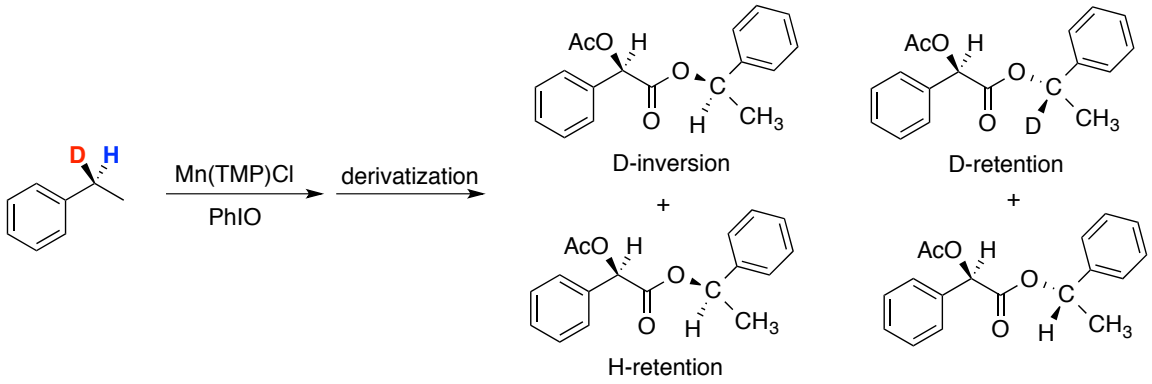


Figure S8. Calibration curve for mass spectral estimation of deuterium content of 1-phenylethyl *O*-acetylmandelate according to White's method.[15]

Scheme S1. Analysis of enantiomers by White's method[3]



An example of determining contents of 4a-4b in reaction mixture (See Figure S9 for detailed GC spectra).



1. Ratio of left peak to right peak = 45.6 : 54.4 (determined by integration of two peaks Figure S10a.
2. 105/106 in left peak = 0.390 (Figure S10b) Determined by mass extraction of 105 and 106 ions
3. D% in left peak = 82% Determined by calibration curve.
4. 105/106 in right peak = 0.338 (Figure S10c) Determined by mass extraction of 105 and 106 ions
5. D% in right peak = 85% Determined by calibration curve.
6. D-inversion content = 45.6% * 0.82 = 37.4%
7. H-retention content = 45.6% * (1-0.82) = 8.2%
8. D-retention content = 54.4% * 0.85 = 46.2%
9. H-inversion content = 54.4% * (1-0.85) = 8.2 %

Net retention% = (46.2 + 8.2 -37.4 -8.2) * 100%= 8.8%

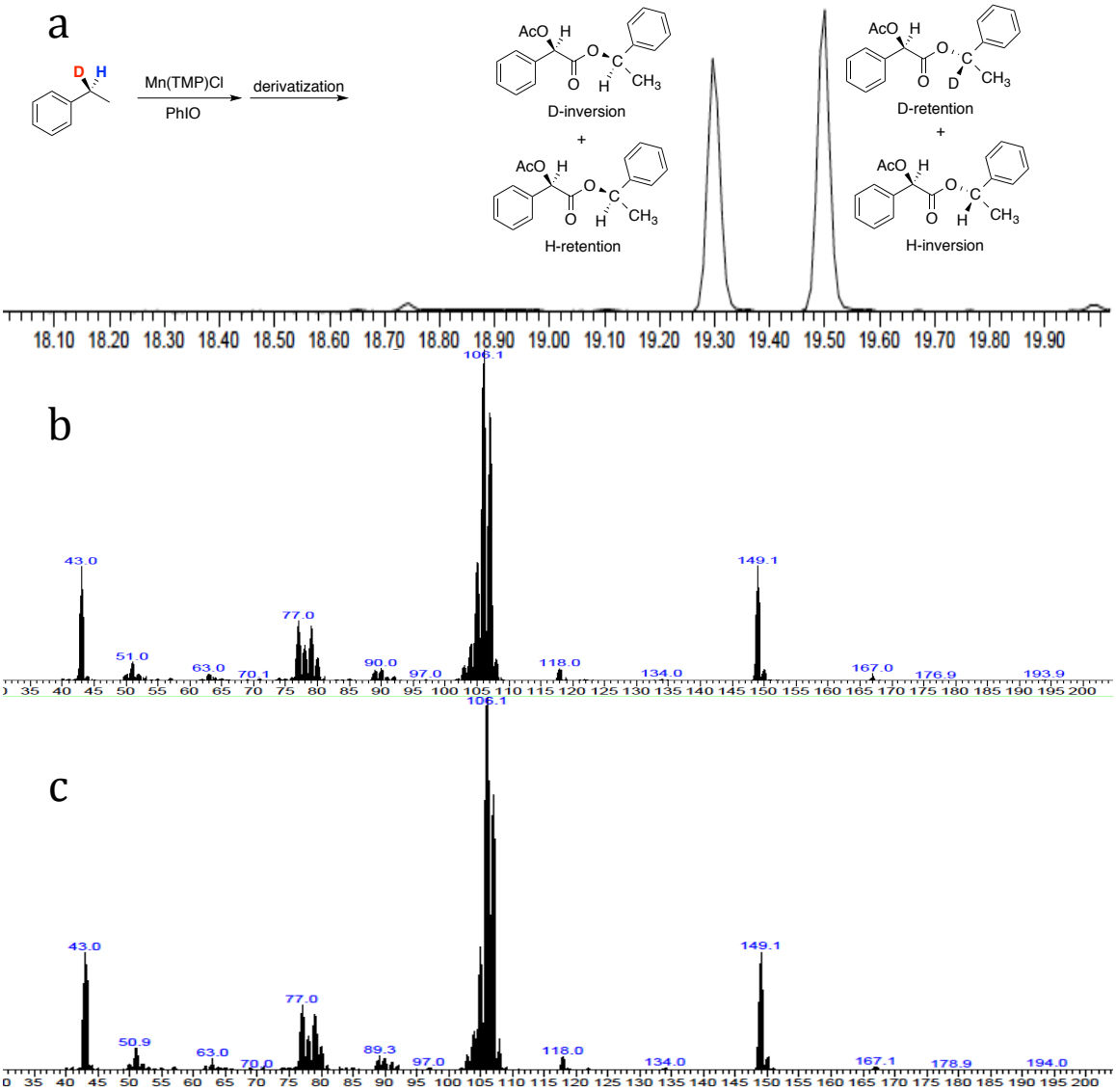


Figure S9. An example of **4** hydroxylation with manganese porphyirin as catalyst (Mn(TMP)Cl as an example)

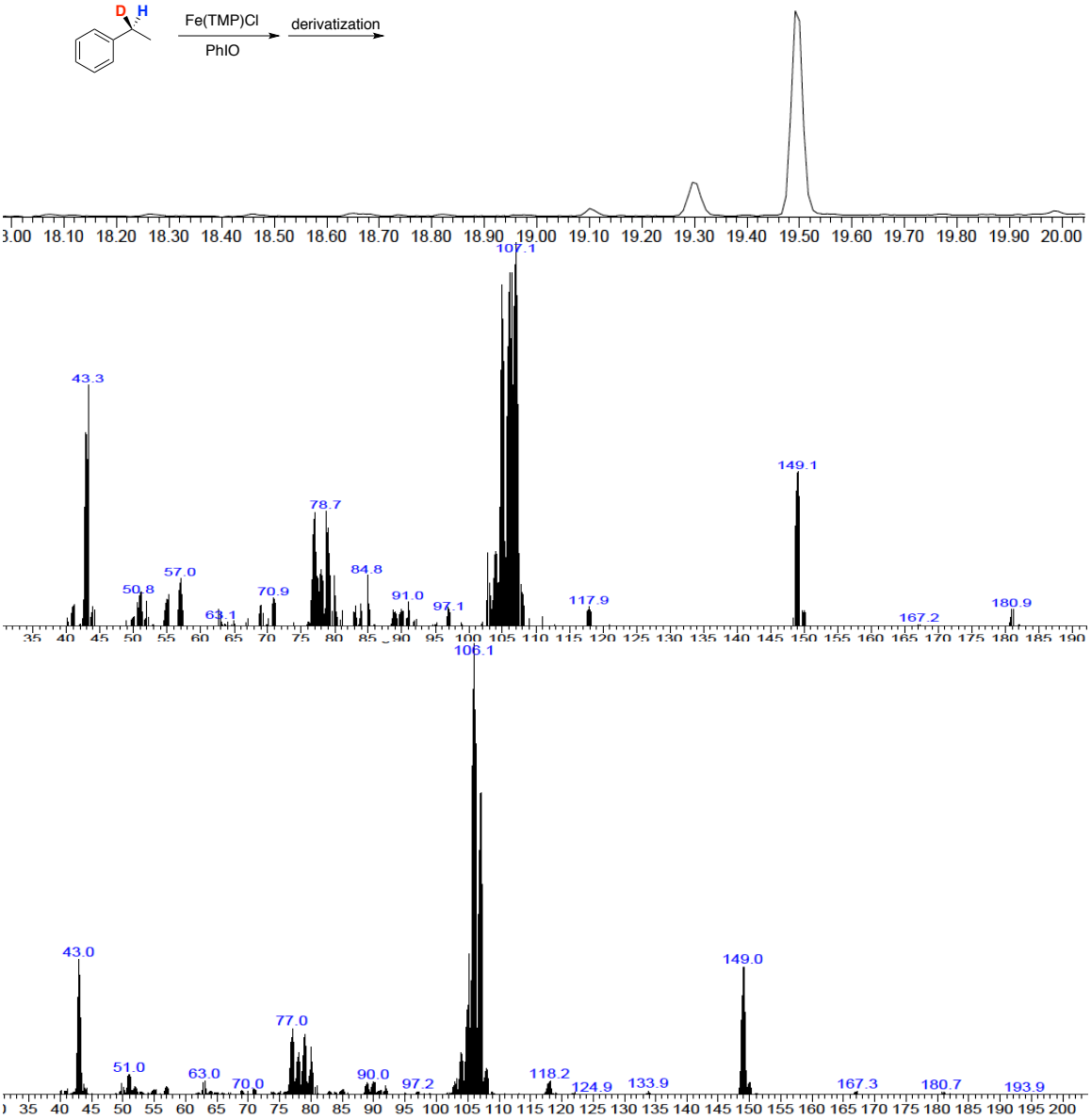


Figure S10. An example of **4** hydroxylation with iron porphyrin as catalyst (Fe(TMP)Cl as an example).

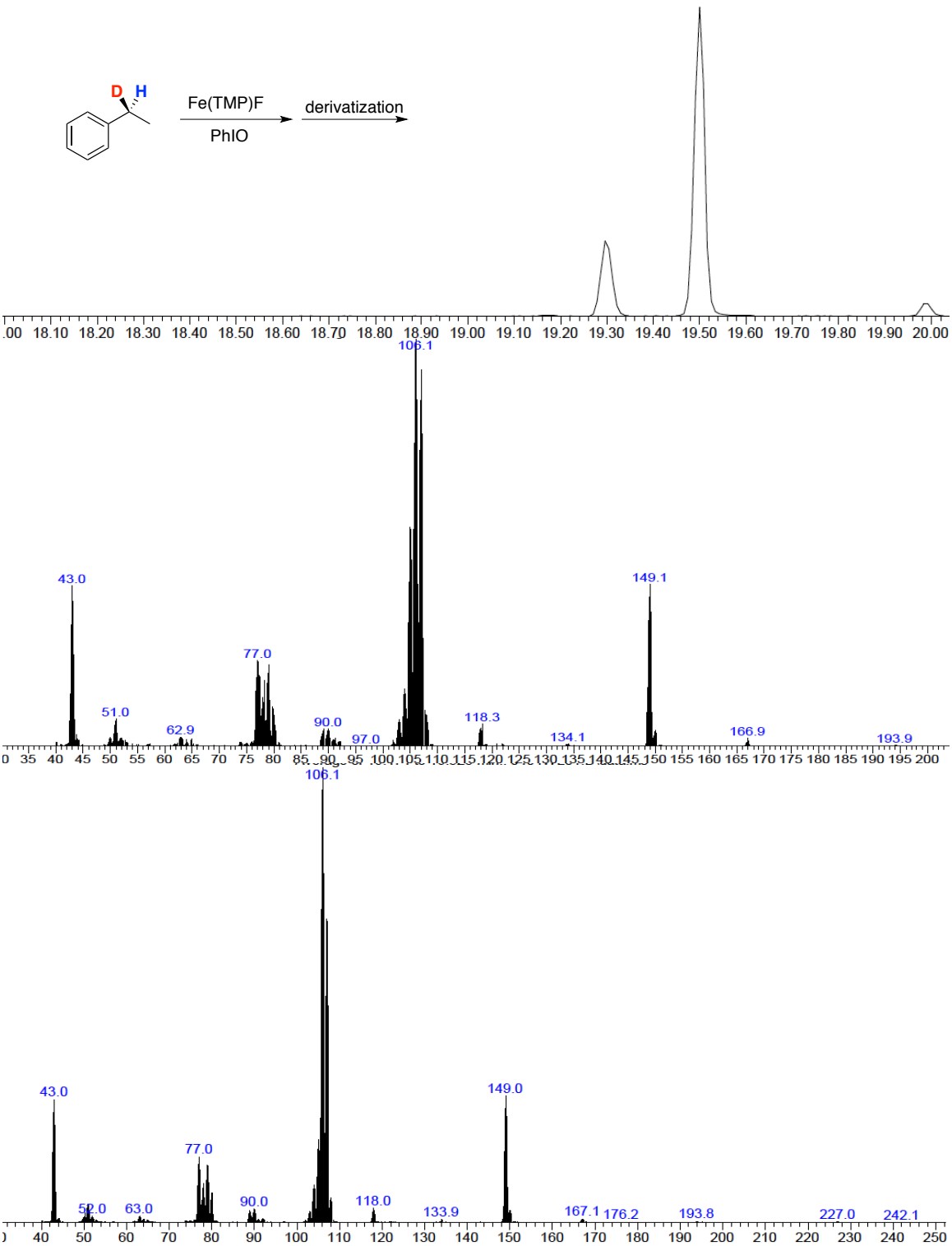


Figure S11.An example of **4** hydroxylation with fluoride-coordinated iron porphyrin as catalyst (Fe(TMP)F as an example).

Table S2. Rebound kinetic barriers under the influence of the solvent dielectric constant (1.0, 2.0, 8.9, 20.0, and 40.0). The unit for barriers is kcal/mol.

Ea(1-L → 1,2-TS-L)

ε	H_2O	Py	F^-	OH^-(TPFPP)	OH^-	OH^-(TPP)	O^{-2}
1.0	4.0	4.0	5.2	4.6	5.3	5.0	--
2.0	3.4	4.1	5.9	5.2	6.2	6.1	--
8.9	3.5	4.5	6.5	5.8	7.4	7.7	--
20.0	3.7	4.6	6.7	6.0	7.7	8.1	--
40.0	3.8	4.7	6.7	6.1	7.9	8.2	--

Ea(1-L → 1,2-TS-H)

ε	H_2O	Py	F^-	OH^-(TPFPP)	OH^-	OH^-(TPP)	O^{-2}
0.0	1.0	2.0	3.1	4.3	4.5	4.5	5.4
2.0	1.5	2.3	4.2	5.1	5.8	5.9	6.8
8.9	2.1	2.9	5.4	6.1	7.5	8.2	8.1
20.0	2.3	3.1	5.7	6.4	7.9	8.9	8.1
40.0	2.4	3.2	5.8	6.5	8.1	9.2	8.0

Coordinates for the optimized transition states

1,2-TS-L-H_2O

O1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	2.6679599491
Mn3	1.3047304267	0.0000000000	-1.1897127422
N4	1.0130915758	1.9318188338	-1.6601276906
N5	2.7692646222	0.5328890730	0.0840068475
N6	1.7169518929	-1.9371800422	-0.8491402860
N7	0.0762771434	-0.5443008880	-2.7164658723
C8	2.6190752883	2.9807954050	-0.1172070882
C9	3.3799819737	-1.6887364894	0.9486006651
C10	0.1479995451	-2.9855675718	-2.4328814670
C11	-0.6808558194	1.6821399993	-3.4338096552
C12	3.1301700141	1.8192176720	0.4376409194
C13	3.4691283857	-0.3061692956	0.9308725210
C14	2.5593933093	-2.4418218598	0.1231125576
C15	1.0924601956	-3.0299921132	-1.4194681880
C16	-0.3332477067	-1.8269887460	-3.0206867496
C17	-0.7124558777	0.2978824429	-3.4750128882
C18	0.1285312401	2.4348420121	-2.5972115169
C19	1.6372123830	3.0273419147	-1.0944017531
C20	1.1191160588	4.2342208929	-1.6731504700
C21	0.1870476061	3.8687679254	-2.5981445223
H22	1.4404396682	5.2306579341	-1.4009169236
H23	-0.4090024817	4.5048556737	-3.2386908159
C24	-1.5920637708	-0.4751911778	-4.3088134571
C25	-1.3573350213	-1.7869201194	-4.0290592837
H26	-2.3002021081	-0.0534664715	-5.0094588707
H27	-1.8345168047	-2.6604996445	-4.4525477211
C28	4.3112046268	0.4688434712	1.7995348438
C29	4.1036908945	1.7797393721	1.4939459331
H30	4.9708681411	0.0493735216	2.5472564884
H31	4.5578759448	2.6541093068	1.9406119646
C32	1.5679979630	-4.2371548581	-0.8052294207
C33	2.4726362637	-3.8741869170	0.1475055028
H34	1.2417414351	-5.2320356207	-1.0771444322
H35	3.0386317341	-4.5110917448	0.8139419674
H36	-0.2606386962	-3.9292890769	-2.7769719999
H37	3.9944962084	-2.2217704111	1.6657919407
H38	3.0082254978	3.9251627949	0.2472793956
H39	-1.3418062390	2.2193894762	-4.1050818856
H40	-0.3594830163	0.8932453812	0.1223533251
O41	2.8529943156	0.0014516664	-2.7309945701
H42	0.6182619001	-0.8864228087	2.6495195497
H43	0.4450110854	0.9614892857	2.8908598610
H44	-1.0764938596	-0.1019046469	2.6262089347
H45	3.6807028006	-0.3974539272	-2.4245926633
H46	2.5577871145	-0.5080377489	-3.5005131217

1,2-TS-H-H_2O

O1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	3.0717827174
Mn3	0.2561329794	0.0000000000	-1.7958015175
N4	0.3478566311	-2.0169174325	-1.9892600386
N5	-1.7007985211	-0.0564170445	-2.2454887933
N6	0.2346994304	2.0174368802	-2.0100375873
N7	2.2560709255	0.0562514818	-1.5655872216
C8	-2.0324780822	-2.4947512844	-2.3737233428
C9	-2.1702445322	2.3589914226	-2.3850910365
C10	2.5906044456	2.4933884208	-1.4878568039
C11	2.7224552030	-2.3573957114	-1.4479207611
C12	-2.4805879185	-1.1843145986	-2.4262810195
C13	-2.5434482909	1.0247095845	-2.4295357256
C14	-0.8798979903	2.8163655291	-2.1711080899
C15	1.2865441777	2.8766623859	-1.7577078526
C16	3.0347558317	1.1827515526	-1.3943413277
C17	3.0943302219	-1.0233941018	-1.3744962096
C18	1.4429677082	-2.8144096139	-1.7193380503
C19	-0.7198888202	-2.8772159578	-2.1493542462

C20	-0.2743062426	-4.2376068802	-2.0267966457
C21	1.0606558555	-4.1989923151	-1.7595010372
H22	-0.9152043415	-5.1030566090	-2.1259254473
H23	1.7371303205	-5.0270102507	-1.5954060276
C24	4.4253931800	-0.5629073050	-1.0947340920
C25	4.3888305419	0.7995896704	-1.1074778451
H26	5.2727697136	-1.2104119558	-0.9134605120
H27	5.2005131568	1.4944396228	-0.9383998066
C28	-3.8745714858	0.5624572752	-2.7009061114
C29	-3.8358122093	-0.7998153567	-2.6995400488
H30	-4.7223145684	1.2099448920	-2.8790822253
H31	-4.6456127900	-1.4948728804	-2.8763416950
C32	0.8286033754	4.2379486047	-1.8106943790
C33	-0.5087693898	4.2007614136	-2.0665278487
H34	1.4603161263	5.1034091443	-1.6618233294
H35	-1.1966141339	5.0293584434	-2.1697742316
H36	3.3186746694	3.2799119965	-1.3231347482
H37	-2.9491567185	3.1005690553	-2.5254754664
H38	-2.7674790362	-3.2800150621	-2.5126488587
H39	3.4911477094	-3.1007285670	-1.2681362693
H40	-0.9491132810	-0.0292122941	0.2063994592
H41	1.1491779262	-0.7630800636	-4.3275796757
O42	0.6189701885	-0.0035375062	-4.0473710830
H43	1.0908221670	0.7883943455	-4.3418823150
H44	-0.4645236159	-0.9576365391	3.2747208290
H45	1.0650688751	0.0489291606	2.8917375034
H46	-0.5499558715	0.9110818321	3.2721720240

1,2-TS-L-Py

Mn1	0.0000000000	0.0000000000	0.0000000000
O2	0.0000000000	0.0000000000	1.7925932541
C3	1.9154259105	0.0000000000	3.4615344005
N4	-2.0213363493	-0.1179154121	-0.0402574021
N5	-0.1191332149	1.9985392770	-0.1045351816
N6	1.9938269410	0.1232459626	-0.1318735959
N7	0.0981432808	-1.9932650133	-0.0031938089
C8	-2.5540732979	2.2509999962	-0.3955509531
C9	2.2671011761	2.5512409118	0.1258162624
C10	2.5197634795	-2.2698580359	-0.3265214975
C11	-2.2720059552	-2.5159535625	0.4064639086
C12	-1.2624346644	2.7513376997	-0.2942893808
C13	0.9239136173	2.8950221609	0.0280411518
C14	2.7614920596	1.2577353538	0.0232743177
C15	2.8716448640	-0.9285706306	-0.2691062362
C16	1.2324482831	-2.7602990660	-0.1518956483
C17	-0.9348634302	-2.8656053791	0.2713668347
C18	-2.7773660863	-1.2352822249	0.2269563690
C19	-2.9051306327	0.9185806850	-0.2289942928
C20	-4.2566009912	0.4312170707	-0.1113962582
C21	-4.1770924883	-0.8935071100	0.1926144115
H22	-5.1420125520	1.0425039111	-0.2243542951
H23	-4.9846934084	-1.5922424592	0.3658095308
C24	-0.4338217139	-4.2127766510	0.2881355383
C25	0.8981551023	-4.1495623187	0.0035249929
H26	-1.0379032081	-5.0900513174	0.4775810720
H27	1.6062431666	-4.9633185418	-0.0740064989
C28	0.4195242615	4.2360790188	-0.0616788965
C29	-0.9240643211	4.1463545999	-0.2829993726
H30	1.0274079370	5.1276742258	0.0154182335
H31	-1.6363741110	4.9499938407	-0.4110952437
C32	4.2244686799	-0.4363271456	-0.2364204578
C33	4.1573508455	0.9087223684	-0.0337077245
H34	5.1045326704	-1.0571755016	-0.3340921910
H35	4.9715463814	1.6155097693	0.0554984063
H36	3.3209012699	-2.9937392708	-0.4295398538
H37	2.9853223609	3.3582826355	0.2233536002
H38	-3.3563260277	2.9678676979	-0.5336830580
H39	-2.9799859570	-3.3128245799	0.6071905783
H40	-0.2753563487	0.8626955137	2.1398087708
H41	2.3205459623	-0.8964453832	3.0133370807

H42	2.3898497978	0.9557575877	3.2709055744
H43	1.1962937689	-0.0911428432	4.2656098808
C44	-0.8722305311	-0.9269564973	-2.8272392694
C45	0.6766831549	0.7879405392	-2.9157345087
C46	-0.9378971930	-0.9958399346	-4.2143644234
H47	-1.4646586780	-1.5864683747	-2.2061809286
C48	0.6655015802	0.7834314062	-4.3060259176
H49	1.3042020360	1.4768623558	-2.3646629511
C50	-0.1565230340	-0.1245643681	-4.9710257521
H51	-1.5924325086	-1.7216128630	-4.6848680965
H52	1.2929896428	1.4814835517	-4.8497198225
H53	-0.1871219874	-0.1527650827	-6.0560177372
N54	-0.0799620110	-0.0501197551	-2.1829022536

1,2-TS-H-Py

Mn1	0.0000000000	0.0000000000	0.0000000000
O2	0.0000000000	0.0000000000	1.7877749824
C3	0.7482405603	0.0000000000	4.8002695094
N4	-1.9355911905	-0.5069770767	-0.1497217711
N5	-0.5049628023	1.9452051595	-0.1174720814
N6	1.9374582672	0.5102165660	-0.0023863289
N7	0.5012393025	-1.9501061954	-0.0938455695
C8	-2.9234941020	1.7233513250	-0.4910721489
C9	1.7000135544	2.9360832041	0.3270269417
C10	2.9470478799	-1.7235388815	-0.1952052297
C11	-1.7328812983	-2.9445186724	0.1290316471
C12	-1.7641867402	2.4665120891	-0.3210159177
C13	0.3273627169	3.0157601492	0.1356323454
C14	2.4465276510	1.7687777282	0.2385580790
C15	3.0158904833	-0.3424657315	-0.0800926983
C16	1.7758420792	-2.4654636198	-0.1522969113
C17	-0.3486205221	-3.0210570090	0.0740228360
C18	-2.4680648770	-1.7755146073	-0.0120726882
C19	-3.0019714019	0.3427022116	-0.3752957896
C20	-4.2233379670	-0.4118032781	-0.3863286977
C21	-3.8963306718	-1.7134722384	-0.1414453082
H22	-5.2050746985	0.0140663989	-0.5457239830
H23	-4.5559083049	-2.5681879140	-0.0729282515
C24	0.4117015526	-4.2421338524	0.0964139784
C25	1.7205903734	-3.9010672453	-0.0627293204
H26	-0.0160711116	-5.2289394263	0.2091670976
H27	2.5846140723	-4.5512738368	-0.0942836290
C28	-0.4278310089	4.2382828180	0.0744160294
C29	-1.7132320329	3.9011400726	-0.2287772969
H30	-0.0118513553	5.2248237850	0.2304868464
H31	-2.5660008964	4.5544907629	-0.3574513778
C32	4.2337258185	0.4055253020	0.0782538233
C33	3.8817825823	1.7045783499	0.2955498719
H34	5.2258501622	-0.0249651250	0.0495004072
H35	4.5278926529	2.5552613463	0.4673532272
H36	3.8835372569	-2.2690293135	-0.2362056212
H37	2.2361014600	3.8617347998	0.5074102825
H38	-3.8493387220	2.2657614926	-0.6495948708
H39	-2.2836289393	-3.8724495217	0.2338690723
H40	-0.8934862865	0.0982387842	2.1549302959
H41	1.6524712497	-0.3082598499	4.2920195492
H42	0.5811136473	1.0489719592	5.0106527998
H43	0.1002180953	-0.7455040422	5.2440877836
C44	-0.4310974754	-1.0087461480	-2.9543516995
C45	0.6718030617	1.0212680201	-2.8992818908
C46	-0.3835132057	-1.0461647431	-4.3437859101
H47	-0.8928076994	-1.8091152537	-2.3897133484
C48	0.7607409676	1.0598434904	-4.2866994098
H49	1.0773404462	1.8201334681	-2.2906025856
C50	0.2241574214	0.0066934907	-5.0256138099
H51	-0.8153891709	-1.8882347634	-4.8739172028
H52	1.2433515321	1.9020171703	-4.7711327896
H53	0.2788545145	0.0065239509	-6.1101448525
N54	0.0867557240	0.0057730194	-2.2390189788

1,2-TS-L-OH-TPFPP

C1	0.0000000000	0.0000000000	0.0000000000
O2	0.0000000000	0.0000000000	2.4554930413
Mn3	1.4859597976	0.0000000000	3.5626915794
N4	1.5412151755	-2.0334386791	3.4656924937
N5	2.7748294671	0.1093600749	2.0097771736
N6	1.3520516304	2.0178005995	3.5911418077
N7	0.2616543372	-0.1231255099	5.1798083966
C8	3.0721393537	-2.2990607531	1.5529832067
C9	2.8276691941	2.5577023438	1.6984144575
C10	-0.1242811319	2.2800704516	5.5501393055
C11	0.1661288313	-2.5684251878	5.4458345814
C12	3.2983120928	-0.9463436583	1.3009713475
C13	3.1919649505	1.2524866639	1.3699894899
C14	1.9690695894	2.8970928426	2.7448982354
C15	0.6373119650	2.7670279350	4.4877697105
C16	-0.2850623471	0.9293568185	5.8592784108
C17	-0.1500758366	-1.2608008060	5.8168876315
C18	0.9605003615	-2.9098786433	4.3500811982
C19	2.2650998332	-2.7908940436	2.5806360852
C20	2.1074735867	-4.1890470373	2.8933898369
C21	1.3063882733	-4.2615219551	3.9878441945
H22	2.5672738578	-5.0031330461	2.3526839017
H23	0.9832963183	-5.1464280616	4.5153676033
C24	-0.9940993229	-0.9144199118	6.9383078896
C25	-1.0762210834	0.4382889577	6.9652818573
H26	-1.4622127456	-1.6224290525	7.6055318892
H27	-1.6214637309	1.0577721917	7.6614651844
C28	4.0404289282	0.9051798896	0.2578298247
C29	4.1048581971	-0.4501476773	0.2141900499
H30	4.5144528313	1.6136130865	-0.4049123705
H31	4.6411380669	-1.0664438676	-0.4917598270
C32	0.7989247144	4.1690816061	4.1844339163
C33	1.6192103204	4.2497000619	3.1065407217
H34	0.3419444202	4.9788883420	4.7331126789
H35	1.9675649850	5.1379093447	2.6009643094
H36	-0.3543422933	-0.8964347937	2.3654482173
O37	2.8460094890	0.0115837797	4.7811744656
H38	3.6972731809	0.0662939234	4.3225420990
C39	-0.7982014717	3.2781132223	6.4336183869
C40	-0.1475959323	3.8017672350	7.5534076164
C41	-2.0965747876	3.7218220956	6.1747556097
C42	-0.7610075572	4.7329122804	8.3872426805
C43	-2.7297628865	4.6524752076	6.9941154357
C44	-2.0568493552	5.1579725919	8.1038077034
C45	-0.3769025566	-3.6787996427	6.2824591325
C46	-1.5088365551	-4.3966960557	5.8901989484
C47	0.2270682064	-4.0375009771	7.4902942445
C48	-2.0257809422	-5.4328661238	6.6624639005
C49	-0.2735251055	-5.0688086651	8.2808453051
C50	-1.4035252493	-5.7675016461	7.8626300489
C51	3.3618001862	3.6635595632	0.8499952471
C52	4.5717703949	4.2947023783	1.1445884496
C53	2.6605617827	4.1062920962	-0.2740277401
C54	5.0706429935	5.3280624243	0.3560427336
C55	3.1385022158	5.1374236733	-1.0777643150
C56	4.3489775631	5.7487259770	-0.7584669994
C57	3.7249186222	-3.2923667165	0.6507511364
C58	5.0256642632	-3.7451988529	0.8794679040
C59	3.0487342525	-3.8065814481	-0.4577324816
C60	5.6357174350	-4.6756061025	0.0425422336
C61	3.6362576449	-4.7385669605	-1.3083788322
C62	4.9355321252	-5.1726524850	-1.0541683006
F63	-2.1276108664	-4.0911922987	4.7418320675
F64	-3.1113908128	-6.1021973351	6.2623314817
F65	-1.8903749990	-6.7581776953	8.6119462501
F66	0.3229880094	-5.3927557855	9.4319069724
F67	1.3151508675	-3.3834938638	7.9124191839
F68	1.4937270221	3.5333518057	-0.6023757666
F69	2.4474420666	5.5416265743	-2.1476715375
F70	5.2835771445	3.9082681376	2.2103566181

F71	6.2318683816	5.9145346230	0.6614626953
F72	4.8177315970	6.7374701366	-1.5215827444
F73	1.7980417743	-3.4009564419	-0.7244175916
F74	2.9663897292	-5.2155283373	-2.3615594129
F75	5.5097099775	-6.0649558741	-1.8625290052
F76	6.8815491973	-5.0925488121	0.2859316469
F77	5.7176679375	-3.2839497453	1.9282701348
F78	-2.7640262144	3.2509393953	5.1146631378
F79	-3.9732754231	5.0606174343	6.7223026612
F80	-2.6540297649	6.0503703596	8.8960166376
F81	-0.1163077003	5.2183056390	9.4525810474
F82	1.0975743522	3.4089682509	7.8459734793
H83	-1.0813931366	-0.0396389336	-0.0039317670
H84	0.4892536630	0.9619700772	-0.0523901412
H85	0.5690900982	-0.9030363537	-0.1800910283

1,2-TS-H-OH-TPFPP

C1	0.0000000000	0.0000000000	0.0000000000
O2	0.0000000000	0.0000000000	2.3574582960
Mn3	0.5131103085	0.0000000000	4.1762760890
N4	-1.3972210292	-0.4865710130	4.6892876289
N5	0.9750604314	-1.9815977945	4.0465229676
N6	2.3787354842	0.4735017216	3.5188248355
N7	0.0580013319	1.9653153069	4.3534855746
C8	-1.1942506393	-2.9476626792	4.7161739489
C9	3.2798022104	-1.7932892840	3.1814513204
C10	2.2304887408	2.9258075245	3.6873074842
C11	-2.3011353829	1.7842292180	5.0422112993
C12	0.1330456312	-3.0372097200	4.2899956338
C13	2.1539718733	-2.5129873318	3.5868230852
C14	3.3696583243	-0.4002829621	3.1645281142
C15	2.8986790140	1.7329778143	3.4059823468
C16	0.9056626163	3.0139084999	4.1174929073
C17	-1.1479899992	2.5009958134	4.7160300455
C18	-2.3896117614	0.3906793972	5.0499479592
C19	-1.8855255596	-1.7507787171	4.9130083272
C20	-3.2389395003	-1.6653721485	5.4018527815
C21	-3.5507910021	-0.3461869652	5.4825434869
H22	-3.8593245684	-2.5100156563	5.6615399114
H23	-4.4750097719	0.0964793682	5.8224572543
C24	-1.0578914261	3.9418631782	4.7129925236
C25	0.2110177956	4.2583568592	4.3510069325
H26	-1.8668026977	4.6151262217	4.9540009837
H27	0.6438624478	5.2416299866	4.2399636811
C28	2.0602015764	-3.9520562018	3.5690716834
C29	0.8146351962	-4.2754599830	4.0040229813
H30	2.8460212750	-4.6219960985	3.2522919548
H31	0.3848728310	-5.2607702045	4.1092588179
C32	4.2670494535	1.6533818727	2.9487298266
C33	4.5570824433	0.3362744489	2.7966723189
H34	4.9137380214	2.5002515806	2.7719202941
H35	5.4888564477	-0.1057725423	2.4754684758
H36	-0.9454047246	-0.2110246895	2.3182794190
O37	1.0562872247	0.0305023226	5.9434856779
H38	1.4471736308	-0.8086177557	6.2245945517
C39	2.9898194238	4.2000922121	3.5148871757
C40	3.7200475361	4.7505171262	4.5708731496
C41	3.0007982363	4.8825994079	2.2967175774
C42	4.4356891668	5.9360417892	4.4254662994
C43	3.7081659102	6.0697147643	2.1282226721
C44	4.4274821684	6.5957392637	3.1986919535
C45	-3.5228787292	2.5563288839	5.4155559790
C46	-4.5686174430	2.7325688147	4.5058581071
C47	-3.6722146231	3.1242743193	6.6834290598
C48	-5.7192140292	3.4425826783	4.8362815736
C49	-4.8125985863	3.8415109511	7.0358995155
C50	-5.8386475902	3.9989295142	6.1074284747
C51	4.4790152308	-2.5701898357	2.7500963529
C52	5.3919636945	-3.0644667556	3.6845496726
C53	4.7317650533	-2.8286297800	1.4010353997

C54	6.5157489647	-3.7896540247	3.2985638962
C55	5.8487153274	-3.5518728971	0.9911258490
C56	6.7420492438	-4.0325416163	1.9457690332
C57	-1.9302159481	-4.2220407664	4.9632499225
C58	-1.7412182168	-4.9558556306	6.1368495696
C59	-2.8352783112	-4.7282977058	4.0270201574
C60	-2.4216837278	-6.1467239965	6.3756696898
C61	-3.5289325796	-5.9155391324	4.2442900264
C62	-3.3189036077	-6.6255530204	5.4241851497
F63	-4.4770285338	2.2115318594	3.2752832954
F64	-6.7029552198	3.5951569430	3.9443872669
F65	-6.9362775821	4.6825098680	6.4354946901
F66	-4.9294651379	4.3734133596	8.2562291514
F67	-2.7049370084	2.9832390932	7.5962132451
F68	3.8867916466	-2.3778712969	0.4652459459
F69	6.0665060836	-3.7873856983	-0.3062356812
F70	5.1959588012	-2.8415209167	4.9904852447
F71	7.3745903277	-4.2493208901	4.2133056186
F72	7.8157017027	-4.7263831212	1.5640468598
F73	-3.0504665266	-4.0666899371	2.8820202527
F74	-4.3875694769	-6.3777329319	3.3304133703
F75	-3.9774593118	-7.7648304800	5.6429000235
F76	-2.2225176731	-6.8273135678	7.5082118658
F77	-0.8883954229	-4.5148496890	7.0694732393
F78	2.3183510716	4.3962737890	1.2528174238
F79	3.7006627591	6.7029598914	0.9510431578
F80	5.1098500171	7.7324751569	3.0484857914
F81	5.1273756002	6.4413051990	5.4511729738
F82	3.7440144873	4.1342161283	5.7579924070
H83	1.0684250503	0.1561579960	-0.0007200631
H84	-0.3871611631	-1.0005304040	-0.1415686087
H85	-0.6586436013	0.8501087739	-0.1174299564

1,2-TS-L-OH

O1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	2.3970440162
Mn3	1.4344210233	0.0000000000	-1.1766472529
N4	1.0038776149	1.9476723774	-1.6123665819
N5	2.7680805285	0.6140950003	0.2195075963
N6	1.7872026570	-1.9248274811	-0.6639790334
N7	0.1586424532	-0.6076921932	-2.6416176806
C8	2.5209931559	3.0508978366	-0.0307263490
C9	3.4431217606	-1.5756367241	1.1118326781
C10	0.3392231779	-3.0289979235	-2.3164646109
C11	-0.5507264547	1.5835374842	-3.4832889404
C12	3.0644499421	1.9151559317	0.5552484481
C13	3.4886243925	-0.1878387149	1.0730406618
C14	2.6488350203	-2.3758662761	0.2997526692
C15	1.2373147138	-3.0311072377	-1.2578119570
C16	-0.1536695319	-1.8994290048	-2.9565133589
C17	-0.5553948695	0.1945288883	-3.4872595816
C18	0.1804373274	2.3886953659	-2.6188622272
C19	1.5741470053	3.0600321001	-1.0483011453
C20	1.0633357545	4.2453522590	-1.6914358119
C21	0.2028724386	3.8298932020	-2.6621100508
H22	1.3450820728	5.2570284526	-1.4303114123
H23	-0.3656764433	4.4311044496	-3.3590554278
C24	-1.3437974918	-0.6232283440	-4.3823318324
C25	-1.0960559772	-1.9188642548	-4.0530910954
H26	-1.9980294127	-0.2365374743	-5.1522847935
H27	-1.5049299755	-2.8172309882	-4.4967239689
C28	4.2855899195	0.6321481745	1.9504477298
C29	4.0232544353	1.9297840913	1.6314632186
H30	4.9490481571	0.2480300179	2.7137985244
H31	4.4293151978	2.8274387980	2.0792408866
C32	1.7546937075	-4.2227611251	-0.6295796083
C33	2.6279726053	-3.8183173187	0.3326673188
H34	1.4790144352	-5.2313654949	-0.9073587200
H35	3.2157545145	-4.4261750068	1.0075373262
H36	-0.0028471265	-3.9938053845	-2.6768168069

H37	4.0777765819	-2.0745582626	1.8369886582
H38	2.8709182730	4.0119046268	0.3322359730
H39	-1.1666842527	2.0843263188	-4.2232843374
H40	-0.4192015049	0.8722987036	-0.0008327067
O41	2.7224465836	-0.0195451712	-2.4743790405
H42	0.9995410782	-0.3995365521	2.4682665904
H43	-0.1622857040	1.0560095465	2.5698065962
H44	-0.8441339223	-0.6732952149	2.3837731079
H45	3.5822502253	0.1436423065	-2.0599710771

1,2-TS-H-OH

O1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	2.3220402685
Mn3	0.5423670261	0.0000000000	-1.8205051130
N4	-1.3815484442	0.4226449796	-2.3498405836
N5	0.9395159792	1.9983322005	-1.7047410551
N6	2.4171228924	-0.4090964268	-1.1374232736
N7	0.1517470953	-1.9826389592	-1.9750568548
C8	-1.2593744883	2.8779755713	-2.3618895555
C9	3.2481207697	1.8834057223	-0.8652734093
C10	2.3250304992	-2.8588127247	-1.2376647066
C11	-2.1865803219	-1.8708522713	-2.7126578224
C12	0.0617045416	3.0230339000	-1.9543404959
C13	2.1097948954	2.5695316093	-1.2716059297
C14	3.3840001831	0.5015646094	-0.8094746238
C15	2.9650922234	-1.6525188724	-0.9818084311
C16	1.0215493202	-3.0019261991	-1.6960386240
C17	-1.0281406310	-2.5552332858	-2.3660528900
C18	-2.3393684029	-0.4901521359	-2.7154121422
C19	-1.9180129242	1.6700428058	-2.5558398541
C20	-3.2737058738	1.5381812357	-3.0294354261
C21	-3.5335294884	0.2047484600	-3.1274213974
H22	-3.9268552979	2.3690143727	-3.2621876874
H23	-4.4425705740	-0.2806498320	-3.4568311715
C24	-0.8964431898	-3.9929835673	-2.3474451200
C25	0.3705143833	-4.2685439261	-1.9337272766
H26	-1.6829370011	-4.6861785428	-2.6156765656
H27	0.8372942467	-5.2342776475	-1.7924323398
C28	1.9766640577	4.0055250219	-1.2831207429
C29	0.7121645921	4.2855505453	-1.7051768938
H30	2.7574495112	4.6970229649	-0.9945357298
H31	0.2445187328	5.2527287549	-1.8330749536
C32	4.3281936792	-1.5250009917	-0.5203537191
C33	4.5871755767	-0.1932414329	-0.4132308670
H34	4.9882594411	-2.3576095881	-0.3149774866
H35	5.5033985861	0.2915674688	-0.1023521162
H36	2.8918791981	-3.7679394583	-1.0646642696
H37	4.1034364346	2.4792279531	-0.5632677941
H38	-1.8248944258	3.7859772762	-2.5446578897
H39	-3.0425750971	-2.4651455231	-3.0144745887
H40	-0.9556586886	0.1626073533	0.0047724785
O41	1.1068196133	-0.0237638429	-3.5854919930
H42	1.0627131756	-0.1908584313	2.3196321910
H43	-0.3541463093	1.0130865446	2.4607540141
H44	-0.6834070009	-0.8273321059	2.4598342098
H45	1.4277310111	0.8469291364	-3.8589314931

1,2-TS-L-OH-TPP

C1	0.0000000000	0.0000000000	0.0000000000
O2	0.0000000000	0.0000000000	2.3692680656
Mn3	1.4795735212	0.0000000000	3.4983487814
N4	1.2924235643	-2.0172562966	3.6814254969
N5	2.8042498522	-0.2610437696	1.9970737158
N6	1.5769827603	1.9989314544	3.2364610511
N7	0.2138951972	0.2501128915	5.0657072525
C8	2.6681725349	-2.7228743972	1.7453157883
C9	3.3729652531	2.1125306822	1.5451439436
C10	-0.1233721136	2.6904425329	4.9068377188
C11	-0.0049348585	-2.1049113205	5.7900857489

C12	3.0738220870	-1.4455184806	1.3422459548
C13	3.4438846976	0.7362455432	1.2938124887
C14	2.4849386896	2.6825789924	2.4663213406
C15	0.8558184847	2.9352162415	3.9342393419
C16	-0.3977093858	1.4212968759	5.4301303685
C17	-0.2911175655	-0.7351123201	5.8713886338
C18	0.7473952218	-2.6806581216	4.7597788832
C19	1.9018160893	-2.9646997829	2.8948930292
C20	1.7210535240	-4.2659813896	3.4858597281
C21	1.0302273361	-4.0882896743	4.6437866311
H22	2.1111813468	-5.1868104053	3.0800571665
H23	0.7394879849	-4.8390011976	5.3629499614
C24	-1.2639398713	-0.1653047680	6.7762035180
C25	-1.3456371659	1.1588317910	6.4886806818
H26	-1.8296046218	-0.7230596898	7.5072090046
H27	-1.9845368231	1.8995605845	6.9444463941
C28	4.1425167771	0.1595996156	0.1734117710
C29	3.8953665105	-1.1770196202	0.1897734049
H30	4.7151937573	0.7196281945	-0.5505890451
H31	4.2340670457	-1.9214759475	-0.5140440091
C32	1.3272923398	4.2544340144	3.5889154695
C33	2.3467477913	4.0982556809	2.7041711663
H34	0.9449573095	5.1734114138	4.0062948214
H35	2.9552425071	4.8659941043	2.2506510048
H36	-0.3985950319	-0.8818935177	2.3818865311
O37	2.8220115321	0.0167231504	4.7433524025
H38	3.6614433103	-0.1257261010	4.2823930281
C39	-0.8804599389	3.8646142211	5.4395191722
C40	-0.7396371201	4.2819324054	6.7718967196
C41	-1.7454781276	4.5816982787	4.5981568167
C42	-1.4469604011	5.3847687414	7.2501505480
C43	-2.4554284977	5.6818210542	5.0782500703
C44	-2.3078826950	6.0866546949	6.4055153809
C45	-0.5778634086	-2.9992795062	6.8408974746
C46	-1.5401298883	-3.9697003165	6.5222581376
C47	-0.1708310297	-2.8702598765	8.1775838604
C48	-2.0802708462	-4.7892916696	7.5129213642
C49	-0.7075957311	-3.6932257409	9.1673010770
C50	-1.6643650322	-4.6544823996	8.8382291252
C51	4.2557870177	3.0146232630	0.7456827988
C52	5.6506977375	2.9466037529	0.8867037032
C53	3.7183302176	3.9379987812	-0.1646728397
C54	6.4840466082	3.7817948306	0.1433217838
C55	4.5520825465	4.7702258628	-0.9110263455
C56	5.9372730921	4.6959465629	-0.7581393783
C57	3.1117838209	-3.9042977198	0.9450202671
C58	4.4693211760	-4.2410116025	0.8308585958
C59	2.1645610348	-4.7139486094	0.2991947291
C60	4.8682362128	-5.3523558114	0.0890183131
C61	2.5632331638	-5.8231967351	-0.4457811398
C62	3.9166425137	-6.1457949287	-0.5531602160
H63	-1.0796899131	-0.0354672452	-0.0581284379
H64	0.4962099538	0.9590124716	0.0005459266
H65	0.5786007819	-0.8938527786	-0.1907579268
H66	4.1182871060	5.4743016508	-1.6160697434
H67	2.6408179621	3.9919092563	-0.2922579162
H68	6.5864543549	5.3455972214	-1.3387507345
H69	6.0780060378	2.2390089634	1.5917717815
H70	7.5614355512	3.7198081522	0.2710942470
H71	1.1105146636	-4.4632119283	0.3798612282
H72	1.8156289879	-6.4345034253	-0.9440456515
H73	4.2277821613	-7.0112587162	-1.1317479162
H74	5.9236174500	-5.6013400778	0.0175042367
H75	5.2115382488	-3.6324745900	1.3386827431
H76	-1.8725637613	-4.0694420179	5.4928542495
H77	-2.8306564531	-5.5299605503	7.2493745721
H78	-2.0849773496	-5.2933183848	9.6100675085
H79	-0.3764338287	-3.5839047820	10.1965232500
H80	0.5758312168	-2.1238530892	8.4333657927
H81	-0.0617556319	3.7438627893	7.4279734573
H82	-1.3205803950	5.6984923484	8.2828994348
H83	-2.8590268918	6.9453611407	6.7791183918

H84	-3.1255632367	6.2216666349	4.4146239875
H85	-1.8632473446	4.2638685620	3.5658723599

1,2-TS-H-OH-TPP

C1	-0.0486670061	0.1744912637	0.0684875693
O2	-0.0222091209	0.0015725215	2.3754592501
Mn3	0.5219481821	-0.0076039154	4.2006650321
N4	-1.3864919179	-0.4907251994	4.7060569056
N5	0.9751197252	-1.9883888011	4.0595643083
N6	2.3804872377	0.4628823124	3.5329585376
N7	0.0791325245	1.9599127883	4.3811135942
C8	-1.1412586120	-2.9435110445	4.9326093541
C9	3.2018300628	-1.8102033862	2.9921253640
C10	2.3181733517	2.9063989806	3.8962573947
C11	-2.3436955592	1.7952865606	4.8374652964
C12	0.1381532624	-3.0357444118	4.3637749523
C13	2.0757239832	-2.5211291697	3.4267577361
C14	3.3449512178	-0.4215568407	3.1255908598
C15	2.9664509025	1.7020295041	3.5946034687
C16	0.9514676269	3.0007978999	4.1918058001
C17	-1.1696357658	2.5032915556	4.5500944243
C18	-2.3919940765	0.4024626390	4.9913279985
C19	-1.8290994148	-1.7353712120	5.0986641932
C20	-3.1523184001	-1.6148723031	5.6560630884
C21	-3.5071000537	-0.3050290788	5.5681445684
H22	-3.7287887168	-2.4310717492	6.0647335980
H23	-4.4247286182	0.1577258416	5.8979599200
C24	-1.0835084478	3.9402509757	4.4425559182
C25	0.2255888372	4.2474333246	4.2469823366
H26	-1.9206840582	4.6185579026	4.5087123352
H27	0.6663078486	5.2242884585	4.1146833952
C28	1.9182820291	-3.9497895245	3.3238778022
C29	0.7376429003	-4.2687291775	3.9197618905
H30	2.6222392804	-4.6176709441	2.8507951871
H31	0.2875711101	-5.2450408040	4.0208899013
C32	4.3602968162	1.5890740520	3.2364963289
C33	4.5883064641	0.2855115710	2.9272272953
H34	5.0659837945	2.4060933301	3.2276860056
H35	5.5181117305	-0.1723478319	2.6245119972
H36	-0.9296553877	-0.3388225761	2.3640087637
O37	1.0834917976	-0.0009786115	5.9710693856
H38	1.5430219051	-0.8268430174	6.1769870206
C39	3.1114327685	4.1724737424	3.8491153049
C40	3.3277586261	4.9159773992	5.0194901565
C41	3.6503617913	4.6459791045	2.6427835070
C42	4.0693937714	6.0966990721	4.9857407599
C43	4.3870396370	5.8297272999	2.6087430180
C44	4.6007250295	6.5573012834	3.7803702832
C45	-3.6124619156	2.5587383450	5.0347602704
C46	-4.6908190604	2.3683203991	4.1564617900
C47	-3.7617727231	3.4702064376	6.0913038997
C48	-5.8809674075	3.0751014326	4.3239124675
C49	-4.9537566271	4.1739475213	6.2613036275
C50	-6.0159828077	3.9806529292	5.3770750979
C51	4.3352513607	-2.5693207026	2.3834049379
C52	5.0654965790	-3.5109217161	3.1248730670
C53	4.6967345166	-2.3432953593	1.0460569271
C54	6.1249193252	-4.2081513364	2.5450892823
C55	5.7530956639	-3.0438000147	0.4650316559
C56	6.4707259573	-3.9783451332	1.2127761589
C57	-1.8212425442	-4.2142962284	5.3275553080
C58	-1.2893302972	-5.0155332886	6.3498460172
C59	-2.9914533423	-4.6422759524	4.6815063327
C60	-1.9134746204	-6.2065575353	6.7195772614
C61	-3.6127529485	-5.8356379490	5.0476322372
C62	-3.0765648143	-6.6206373364	6.0691377016
H63	0.9426752931	0.6021651220	0.0878694207
H64	-0.1649995326	-0.8788686339	-0.1494311606
H65	-0.9029500915	0.8334964923	-0.0141849682
H66	-6.9436236859	4.5308683392	5.5089969198

H67	-6.7019814254	2.9198053427	3.6290980556
H68	-4.5852878749	1.6674943697	3.3329814345
H69	-2.9409237672	3.6144563739	6.7873877437
H70	-5.0535928557	4.8708611826	7.0891430617
H71	2.9194360031	4.5548285625	5.9589473713
H72	4.2345587052	6.6552999150	5.9031908552
H73	5.1770654479	7.4781149161	3.7537397733
H74	4.7914685942	6.1852493222	1.6647871965
H75	3.4786487686	4.0849361497	1.7284824173
H76	-0.3863706342	-4.6927589305	6.8604888140
H77	-1.4914590667	-6.8103285449	7.5184335668
H78	-3.4057379192	-4.0385090921	3.8795747213
H79	-4.5139416380	-6.1541843908	4.5305517030
H80	-3.5612802394	-7.5500678074	6.3552285904
H81	4.8055802432	-3.6848875461	4.1648509096
H82	6.6834107608	-4.9283174343	3.1370678932
H83	7.2953254774	-4.5227418118	0.7608419134
H84	6.0139505616	-2.8604932156	-0.5738301439
H85	4.1357386219	-1.6193247761	0.4619853988

1,2-TS-H-O

O1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	2.2795816488
Mn3	1.5672440103	0.0000000000	-1.1820706427
N4	1.1700515772	1.9950330301	-1.5245543774
N5	2.7781365921	0.5203944112	0.3717533185
N6	1.7969427308	-1.9702931977	-0.7144996962
N7	0.2051869550	-0.5076892339	-2.6400377654
C8	2.6351736566	2.9640063835	0.1808848984
C9	3.3847678945	-1.7299688705	1.1345576301
C10	0.3157931759	-2.9409833679	-2.4114976767
C11	-0.3821296214	1.7443001317	-3.4088977920
C12	3.1093978931	1.7874450660	0.7594049324
C13	3.4543361374	-0.3385134411	1.1888061258
C14	2.6099747392	-2.4826183374	0.2508483984
C15	1.2171177898	-3.0274713022	-1.3514104356
C16	-0.1506037860	-1.7689677484	-3.0060624212
C17	-0.4618638821	0.3523082001	-3.4590572728
C18	0.3767648824	2.5008526707	-2.5150209818
C19	1.7412865931	3.0567935427	-0.8871667629
C20	1.2828320140	4.2940729858	-1.4860896650
C21	0.4363183674	3.9489171509	-2.4975422136
H22	1.5800776012	5.2861090974	-1.1678710504
H23	-0.1011897077	4.6012726127	-3.1757060028
C24	-1.2860408749	-0.3967522739	-4.3914508625
C25	-1.0931943258	-1.7145372738	-4.1092514490
H26	-1.9223844290	0.0430911821	-5.1503673040
H27	-1.5381285099	-2.5780623599	-4.5895942245
C28	4.2506665693	0.4127054078	2.1388283699
C29	4.0356786657	1.7315285810	1.8736963388
H30	4.8813044203	-0.0255875716	2.9033195436
H31	4.4560128737	2.5952098827	2.3753487613
C32	1.6809640530	-4.2696729679	-0.7634584656
C33	2.5471686346	-3.9318386437	0.2317096570
H34	1.3743873365	-5.2588747051	-1.0815397768
H35	3.0961224751	-4.5869981245	0.8978299999
H36	-0.0593605536	-3.8789700493	-2.8133818119
H37	3.9851798658	-2.2803789875	1.8545411518
H38	3.0013545094	3.8982948341	0.5989414672
H39	-0.9729720475	2.2953700819	-4.1369074856
H40	-0.3256575310	0.9101088313	0.0003563557
O41	2.7488117439	-0.0078284676	-2.2995371753
H42	0.5330988550	-0.9378358969	2.2896753871
H43	0.5524849022	0.9163284637	2.4383976940
H44	-1.0751379170	-0.0019914125	2.3982636654

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